

An open-source framework for the computational analysis and design of autothermal chemical processes

DE – EE0008326

Iowa State University of Science and Technology

June 1st, 2018 – May 31st, 2020 (NCE requested to May 31st, 2021)

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June 2nd -3rd, 2020

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Overview

Project title

An open-source framework for the computational analysis and design of autothermal chemical processes

Project timeline

Project Start Date: June 1st, 2018
Budget Period End Date: May 31st, 2019
Project End Date: May 31st, 2020
No-cost Extension: May 31st, 2021

Barriers and challenges

- Formulate a chemical kinetic mechanism for biomass autothermal pyrolysis
- Reduce the computational cost to perform scale-up calculations from days to minutes

AMO MYPP Connection

- Advanced sensors, controls, platforms and modeling for manufacturing
- Process intensification
- Process heating

Project budget and costs

Budget	DOE share	Cost share	Total	Cost share %
Overall budget	854,039	214,012	1,068,051	20%
Approved budget (BP-1)	466,268	116,569	582,837	20%
Approved budget (BP-2)	387,771	97,443	485,214	20%
Costs as of 5/31/20	620,329	214,012	834,341	n. a.

Project team and roles

- PI: Alberto Passalacqua (CFD modeling and kinetics)
- Mark Mba-Wright (Reduced-order modeling)
- Robert Brown (Experiments)
- Shankar Subramaniam (Homogeneous modeling and kinetics)

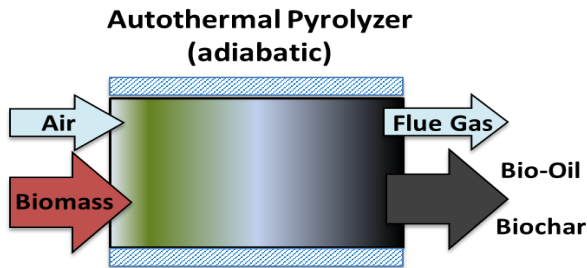
Project objectives

- Scale-up of biomass fast pyrolysis is limited by heat transfer constraints in the pyrolyzers.
- Autothermal biomass fast pyrolysis addresses this limitation by leveraging partial-oxidation reactions of biomass to locally generate heat inside the pyrolyzer.
- **Objective:** develop an experimentally-validated computational tool for autothermal biomass fast pyrolysis to perform design and scale-up of pyrolyzers
 - Difficulty: uncertainty in the kinetics due to partial oxidation processes
- **Relevance to AMO:**
 - Modeling for manufacturing
 - Process intensification

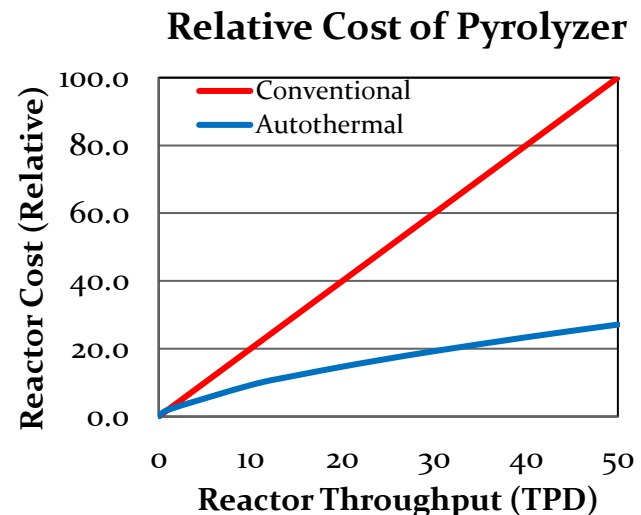
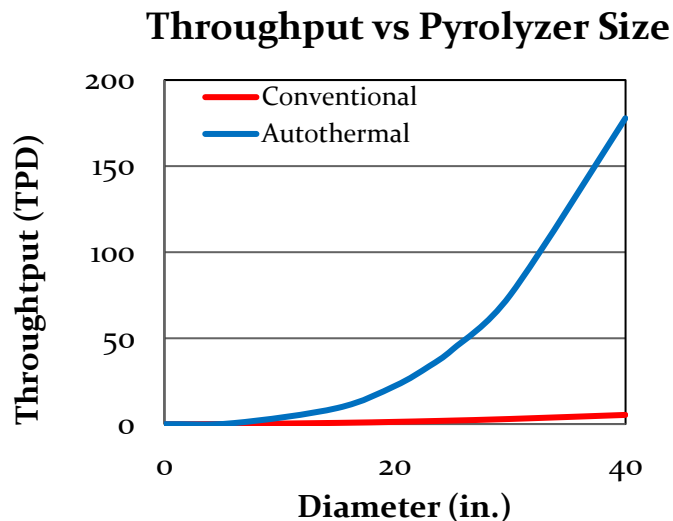
Technical innovation [1]

- Autothermal pyrolysis

- Regular pyrolysis: heat is provided by means of heat transfer
- **Autothermal pyrolysis**: heat is generated by an **exothermal reaction** that happens in parallel to the endothermal one

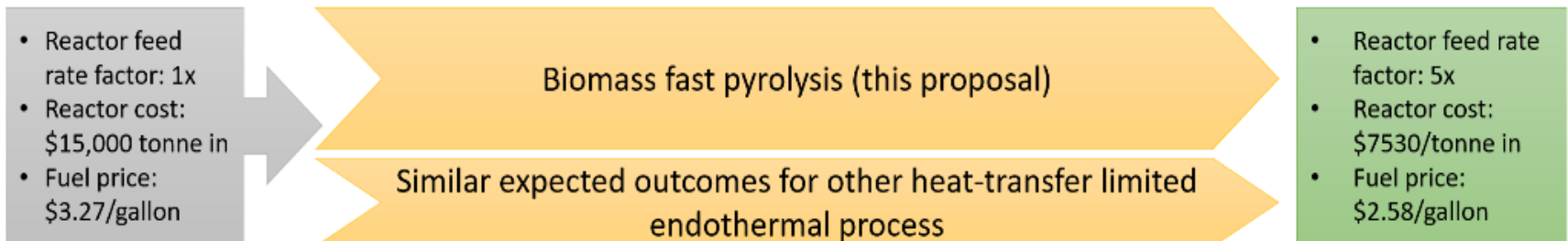


- Heat transfer only scales as **square of reactor diameter** while the energy demand for pyrolysis scales as the **cube of reactor diameter**
- Providing enthalpy of pyrolysis through partial oxidation of products (autothermal pyrolysis) **reduces size and cost of pyrolyzer** compared to a heat transfer-limited reactor



Technical innovation [2]

- Current design and scale-up heavily relies on experimental observations and empiricism
 - Difficult to explore different operating conditions
 - Complex scale-up operations
- The proposed approach will impact the design and scale-up of biomass pyrolizers
 - Systematic investigation of kinetic mechanism
 - Understanding of the role of mixing
 - Formulation of a reduced-order model for reliable scale-up, integrated in already available tools for engineering simulation (OpenFOAM, DWSIM)
 - Demonstration of the reduced-order model to scale-up an autothermal biomass pyrolizer from laboratory scale to 50-250 tpd of processed biomass
- Potential applications to other endothermic chemical processes affected by heat-transfer limitation



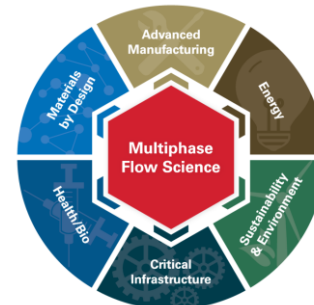
Technical approach [1]

- **Kinetic modeling**
 - Biomass devolatilization
 - Empirical model to reproduce experiments from feedstock composition
 - Char combustion
 - Verification of Langmuir kinetics
 - Gas-phase kinetics
 - Investigation of CRECK detailed mechanism to identify relevant reactions to extract a reduced mechanism for CFD
- **Homogeneous modeling to investigate the role of mixing**
 - PFR model (no mixing) and PaSR model (controlled mixing) with detailed chemical kinetic mechanism for the gas phase
 - Inform CFD model on the relevance of mixing modeling in the non-homogeneous model
- **CFD reactive multiphase model**
 - Implement polydisperse kinetic theory model for the granular phase
 - Implement reduced kinetic mechanism accounting for the relevant reactions for autothermal pyrolysis
 - Use to generate datasets to produce the reduced-order model
- **Experiments to validate kinetic and CFD model**
 - Evaluate kinetics of low-temperature combustion
 - Measure products obtained in a laboratory-scale pyrolyzer to compare with the predictions of the CFD simulations
- **Reduced order model**
 - Kriging model
 - CAPE-OPEN model in DWSIM
 - Validate in scale-up of actual system to pyrolyze 50 – 250 tpd of biomass

Technical approach [2]

- ISU synergic team
 - **Alberto Passalacqua**
 - **Expertise:** development and validation of detailed Euler-Euler CFD models, uncertainty quantification and development of open-source simulation tools. Team-leader for device-scale simulation of the Center for Multiphase Flow Research and Education at ISU. Member of the OpenFOAM Multiphase Technical Committee
 - **Role:** PI and lead of the development and application of the CFD model; contributes to the formulation of the kinetic model
 - **Shankar Subramaniam**
 - **Expertise:** particle-resolved direct numerical simulation, formulation of constitutive laws for multiphase flow, turbulence and mixing modeling. Founding and past Director of the Center for Multiphase Flow Research and Education at ISU
 - **Role:** Co-PI. Formulation of homogeneous model and investigation of mixing; contributes to the formulation of the kinetic model and identification of mixing/transport contribution
 - **Robert Brown**
 - **Expertise:** biomass pyrolysis processes and experimental techniques to collect data from these processes. Director of the ISU Bioeconomy Institute
 - **Role:** Co-PI. Experimental work to collect data for model validation; contributes to the formulation and validation of the kinetic model
 - **Mark Mba-Wright**
 - **Expertise:** formulation of reduced order-models; techno-economic analysis
 - **Role:** Co-PI. Formulation and validation of the reduced-order model

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Bioeconomy Institute



CoMFRE
Multiphase
Flow
Research

Results and accomplishments

Task	Milestones	Status
Task 0	Project management	In progress
Task 1	Formulation of the chemical kinetic model	
Subtask 1.1	The semi-empirical biomass volatilization model has been formulated and successfully reproduces experimental data from the literature.	Completed
Subtask 1.2	The validation of Langmuir kinetics for gas-solid reactions has been completed and satisfactorily reproduces experimental data.	Completed
Subtask 1.3	Key oxidation reactions describing low-temperature combustion have been compared to rate parameters in the literature, and satisfactorily reproduced them, or alternative parameters have been determined through experiments	Completed
Task 2	Homogeneous model	
Subtask 2.1	The adequacy of the PFR model to describe autothermal pyrolysis has been established comparing to experimental measurements concerning the gas-phase reaction.	In progress (90%)
Subtask 2.2	The adequacy of the PaSR model to describe autothermal pyrolysis has been established comparing to experimental measurements concerning the chemical kinetics	In progress (20%)
Task 3	Extension of the Euler-Euler model in OpenFOAM	
Subtask 3.1	The multi-fluid kinetic theory model in OpenFOAM has been extended, and test simulations to ensure its basic functionality have been performed.	Completed
Subtask 3.2	The multi-fluid kinetic theory model has been verified and validated against experiments, and successfully reproduced results from the literature in cold flow cases.	Completed
Subtask 3.3	Chemical kinetic mechanisms selected through the homogeneous model have been translated into input files for the CFD model.	Completed

Results and accomplishments

Task	Milestone	Status
Task 4	Experimental measurements to support model validation	
Subtask 4.1	The experimental setup has been successfully modified and is ready to produce the required experimental data.	Completed
Subtask 4.2	The database of experimental data to validate the chemical kinetic model for low temperature combustion has been completed.	Completed
Subtask 4.3	The database of experimental data to validate the CFD model for low temperature combustion has been completed.	Completed
Task 5	Generation and implementation of the reduced-order model	
Subtask 5.1	The first batch of CFD simulations required to generate the reduced order models have been completed.	In progress (75% complete)
Subtask 5.2	The Kriging reduced order model has been formulated and successfully reproduces the CFD results with an evaluation time of the order of seconds.	In progress (80% complete)
Subtask 5.3	The python code for the reduced order model implementation in DWSIM has been written and successfully reproduces CFD results with evaluation times of the order of minutes.	In progress (75% complete)
Subtask 5.4	The CAPE-OPEN implementation of the ROM in DWSIM has been completed, and successfully reproduces results from the CFD model.	In progress (50% complete)
Subtask 5.5	A complete scale-up study of an autothermal pyrolyzer has been completed using the reduced order model developed in the project.	In progress (10% complete)

Transition plan

- Source code of the model implemented into OpenFOAM will be distributed via GitHub
 - Custom repository for the project
 - Contribution to upstream version of OpenFOAM for long-term maintenance
- Models implemented in DWSIM will be
 - Released via the project GitHub repository
 - Contributed to DWSIM
- Potential for further development
 - Companies developing computational tools for engineering (CFD codes, process simulators)
 - A 50 tpd autothermal pyrolysis demonstration system is being built with private funding